Error Bars for Computational Simulation

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"Prediction is very difficult, especially if it's about the future." – Niels Bohr

The Crew Exploration Vehicle (CEV) Aerosciences Project at Johnson Space Center is responsible for defining the aerodynamic and aerothermodynamic environments that the Orion capsule will experience during reentry. The relevant physical processes involved during reentry from superorbital velocity are shown in figure 1. It is impossible to simultaneously reproduce all of these physical phenomena in any ground test facility because of the tremendous amounts of energy and large scales involved in reentry. Consequently, designers increasingly leverage complex computer simulations to predict what these environments will be. These predictions are then used to design the vehicle without full system-level test data. The obvious question is: how much can the designer trust these predictions? Specifically, how does one define "error bars" for computational simulation?

NASA is not the only agency struggling with this question. As it turns out, the Department of Energy's National Nuclear Security Administration (NNSA) is posed with a similar challenge. The NNSA is responsible for the stewardship of the nation's nuclear stockpile, and is banned by treaty from performing full system-level testing. This question is so vital to the NNSA mission that it created the Predictive Science Academic Alliance Program (PSAAP) to address it.

The Department of Energy awarded five PSAAP centers in 2008. Each center was awarded 5 years of funding to study advanced verification, validation, and uncertainty quantification techniques for coupled multi-physics applications relevant to the NNSA mission. The University of Texas at Austin's Center for Predictive Engineering and Computational Sciences (PECOS) is one of the five PSAAP centers.

The goal of the PECOS center is to develop the next generation of advanced computational methods for predictive simulation of multi-scale, multi-physics phenomena, and to apply these methods to the analysis of vehicles reentering the atmosphere. The Engineering Directorate at Johnson Space Center has partnered with

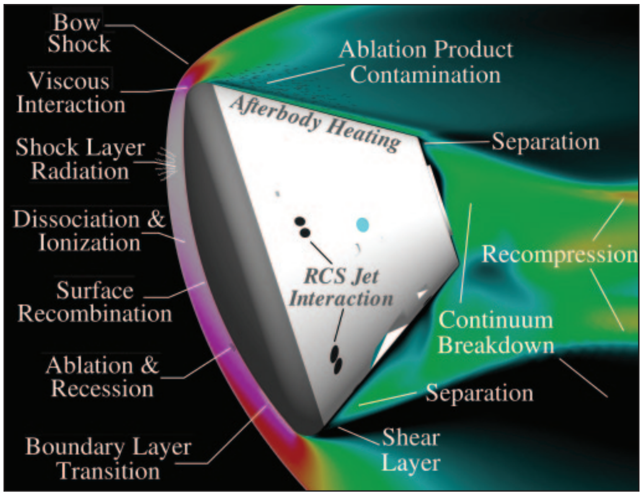

Fig. 1. *Coupled multi-physics relevant in hypersonic entry. The physical scales and energies involved in reentry preclude system-level testing, requiring engineers to increasingly rely on computational predictions in the design process. Understanding the accuracy of these simulations is a critically important and difficult aspect of design. Quantifying the uncertainty in such predications is one focus of NASA's current research.*

PECOS in this goal, and has set up a Space Act Agreement to facilitate the sharing of data and discipline expertise between the two groups.

Today's computational analysts are presented a wealth of mathematical models— each with its own strengths and weaknesses—to describe the phenomena in figure 1. Each model has certain parameters whose values are determined from either theory or experiment. Once the best models and their associated parameters are determined, predictions can be made for the flight environment. Historically, model selection and parameter determination has been somewhat ad hoc, often with single "optimal" parameter values determined for simple configurations, and reported in the literature. A central tenant of the PECOS research is *rigorously informed model selection and parameter determination*. In this approach, the model parameters are instead recast in terms of probabilities, whose most likely values are determined from experimental data. Thus, parameters are defined not by single values but rather through rigorously informed probability distribution functions. In this approach, prediction then does not yield a

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continued

single value, but rather again a distribution function whose width defines the confidence in that prediction.

Additionally, the proliferation of computational models is often a challenge. To simulate the effects of turbulence in a fluid, for example, the analyst must first choose from no fewer than five separate turbulence models, each with its own strengths and weaknesses. Historically, selecting the "optimal" model has been ad hoc, which is unsettling because this choice can have a critical impact on design. The PECOS group introduced the concept of *model plausibility* to address this challenge. Again, the approach is to employ statistical inference techniques to determine which model(s) are most preferred by the available data.

This approach is illustrated in figure 2, where three separate models are employed to predict wall shear stress in a fluid. The result of each prediction is a probability distribution function centered about the most likely value for each model. Further, the models are ranked in terms of plausibility. In this case, Model #3 is dramatically preferred by the data, which would suggest to the analyst that it is the best model to use for prediction in the absence of data.

The project has already contributed some significant findings. As research enters its 4th year, focus is shifting from calibration and model selection to prediction of the coupled multi-physics of reentry using rigorously informed and selected physical models. This is a significant step in the research and will allow designers to use computational predictions with meaningful "error bars" applied because, after all, no computational model will ever be perfect.

"All models are wrong, some are useful." – George Box

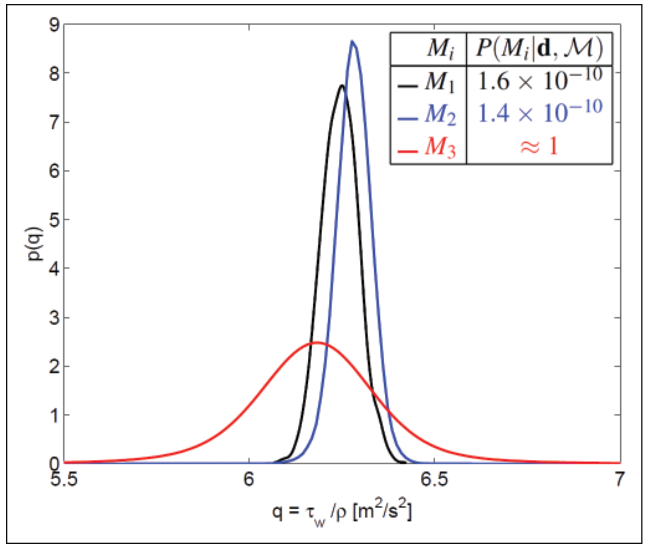

Fig. 2. *Model plausibility and quantity of interest predictions for shear stress in a turbulent flow. Model #3 has the highest uncertainty in the uncertainty in the quantity of interest, but is most likely the correct model given the set of calibration data used. Dr. Todd Oliver of Predictive Engineering and Computational Sciences provided this result.*